Casimir-like tunneling-induced electronic forces

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Abstract. We study the quantum forces that act between two nearby conductors due to electronic tunneling. We derive an expression for these forces by calculating the flux of momentum arising from the overlap of evanescent electronic fields. Our result is written in terms of the electronic reflection amplitudes of the conductors and it has the same structure as Lifshitz's formula for the electromagnetically mediated Casimir forces. We evaluate the tunneling force between two semiinfinite conductors and between two thin films separated by an insulating gap. We discuss some applications of our results.

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1. Introduction

The increased accuracy of experimental studies [1, 2, 3, 4, 5] of the Casimir force [6] between conducting bodies has opened the possibility of exploring new ideas related to the understanding and control of quantum vacuum fluctuations. Research projects on the dynamical Casimir effect [7], Casimir torques [8], or the possible applications of the Casimir forces in the development of micro and nano-electromechanical devices are now under way [9, 10]. Understandig Casimir forces has become fundamental in the investigation of deviations of Newton's Gravitational Law at micrometer dimensions, related to the search for extra dimensions in space-time [11].

The usual Casimir effect may be understood as a force due to the quantum nature of the electromagnetic radiation. In this paper we study another source of quantum forces, namely, the tunnel effect. Particles that are able to tunnel across a barrier have more space available to them. Thus, their contribution to the total energy of a many body system such as two metallic slabs with neighboring surfaces may diminish. As the amount of space gained and the number of particles capable of tunneling depends on the width of the barrier, besides its height, there must be a force that performs work when the width is modified. Since quantum tunneling arises from evanescent electronic

fields, this force is similar to the contributions of evanescent electromagnetic waves to the standard Casimir force.

In this paper we concentrate our attention on conduction electrons in conductors, that is, on massive non-relativistic Fermions. We derive the tunneling force by calculating the flux of momentum between two regions delimited by an arbitrary potential $V(x)$. We express the momentum flux in terms of the Green's function of the system, which we evaluate by means of a scattering method involving amplitude reflection coefficients [12, 13]. This method yields an expression for the tunneling force with a structure that is essentially identical to Lifshitz's formula [14]. We first perform the calculation for a one-dimensional system. We then extend the calculation to the three-dimensional case. Finally, we evaluate the tunneling force for a configuration consisting of two semiinfinite or two thin metallic slabs separated by a thin insulating gap and we discuss some applications of our results.

2. One dimensional systems

The dynamical equation for the wavefunctions of an electronic system may be derived from a Lagrangian density, [15]

$$\mathcal{L} = \frac{\hbar^2}{2m}|\psi_{,z}|^2 + V|\psi|^2 + \frac{i\hbar}{2}\left(\psi\psi^*_{,t} - \psi^*\psi_{,t}\right), \tag{1}$$

for which Euler-Lagrange's equations yields Schrödinger's equation,

$$\partial_t \frac{\partial\mathcal{L}}{\partial(\psi^*_{,t})} + \partial_z \frac{\partial\mathcal{L}}{\partial(\psi^*_{,z})} - \frac{\partial\mathcal{L}}{\partial\psi^*} = i\hbar\psi_{,t} + \frac{\hbar^2}{2m}\psi_{,z,z} - V\psi = 0. \tag{2}$$

The wavefunction carries mechanical properties which may be derived from $\mathcal{L}$: we may obtain a momentum density

$$g = \frac{1}{c}T^0_z = \frac{\partial\mathcal{L}}{\partial\psi^*_{,t}}\psi^*_{,z} + \frac{\partial\mathcal{L}}{\partial\psi_{,t}}\psi_{,z} = \frac{i\hbar}{2}(\psi\psi^*_{,z} - \psi^*\psi_{,z}), \tag{3}$$

where c is the speed of light in vacuum, as well as a momentum flux [16]

$$T^z_z = \frac{\partial\mathcal{L}}{\partial\psi^*_{,z}}\psi^*_{,z} + \frac{\partial\mathcal{L}}{\partial\psi_{,z}}\psi_{,z} - \mathcal{L} = \frac{\hbar^2}{2m}|\psi_{,z}|^2 - V|\psi|^2 - \frac{i\hbar}{2}\left(\psi\psi^*_{,t} - \psi^*\psi_{,t}\right). \tag{4}$$

Consider now an eigenstate ψ_n of the Schrödinger Hamiltonian $\hat{H} = -(\hbar^2/2m)\partial_z^2 + \hat{V}$ corresponding to an energy E_n. From Eq. (4), its contribution to the momentum flux is

$$T^z_z = \frac{\hbar^2}{2m}|\partial_z\psi_n|^2 + (E_n - V)|\psi_n|^2. \tag{5}$$

Within a region $\mathcal{V}$ in which $V(z)$ may be taken as a constant, we can write $E_n - V = \hbar^2k_n^2/2m$, i.e., the kinetic energy of particles with wavenumber k within $\mathcal{V}$. We now sum the contributions (5) over all the occupied orbitals,

$$T^z_z(z) = \frac{\hbar^2}{2m}\sum_n \int dE\,\delta(E - E_n)f(E)\left[k^2|\psi_n(z)|^2 + |\partial_z\psi_n(z)|^2\right], \tag{6}$$

where $f(E_n)$ is the occupation number of orbital n, given in equilibrium by the Fermi-Dirac distribution function, and $k^2 = 2m(E - V)/\hbar^2$. The energy integration and Dirac's δ allow us to write T^z_z in terms of the Green's function of the system,

$$\hat{G}_E(z, z') = \left\langle z\left|\left(E - \hat{H}\right)^{-1}\right|z'\right\rangle = \sum_n \frac{\psi_n(z)\psi^*_n(z')}{E - E_n}, \tag{7}$$

employing the relation $\mathrm{Im}(E^+ - E_n)^{-1} = -\pi\delta(E - E_n)$, where $E^+ = E + i\eta$ with E and $\eta \to 0^+$ real. Substituting this latter relation in (6) and employing (7) we obtain

$$T_z^z(z) = -\frac{\hbar^2}{2\pi m}\mathrm{Im}\int dE\left[k^2 G_{E^+}(z,z') + \partial_z\partial_{z'}G_{E^+}(z,z')\right]_{z'\to z} f(E). \tag{8}$$

Notice that Eq.(8) may be interpreted as

$$T_z^z(z) = \int dE \rho_E^{ef} f(E)(\hbar k)\left(\frac{\hbar k}{m}\right), \tag{9}$$

where $\pm\hbar k$ is the momentum of a particle which moves at velocity $\pm\hbar k/m$, thus contributing the amount $(\hbar k)\hbar k/m$ to the momentum flux, and

$$\rho_E^{ef}(z) = -\frac{1}{2\pi}\mathrm{Im}\left[G_E(z,z') + \frac{1}{k^2}\partial_z\partial_{z'}G_E(z,z')\right]_{z'\to z} \tag{10}$$

plays the role of an effective local density of states.

We now assume that $\mathcal{V}$ has a width L and is bounded on both sides by arbitrary potentials, and we evaluate the Green's function following a scattering approach [12, 13]. Within $\mathcal{V}$, the solution of $(E - H)G_E(z,z') = \delta(z - z')$ may be written as $G_E(z,z') = (2m/\hbar^2)\psi_L(z_L)\psi_R(z_R)/W$, where ψ_L and ψ_R are the two solutions of the Schrödinger-like homogeneous equation $(E - H)\psi = 0$ that satisfy the boundary conditions on the left and the right side of the system respectively, $W = \psi_L\psi_{R,z} - \psi_{L,z}\psi_R$ is their Wronskian, and z_L and z_R are the smallest and the largest among z and z'. We write $\psi_L(z) = e^{-ikz_L} + r_1 e^{ikz_L}$ and $\psi_R(z) = e^{ik(z_R - L)} + r_2 e^{-ik(z_R - L)}$, where r_1 and r_2 are the reflection amplitudes for particles impinging on the left and right boundaries of $\mathcal{V}$, which we assume at $z = 0$ and $z = L$, and we obtain

$$G_E(z,z') = \frac{2m}{\hbar^2}\frac{\left(e^{-ikz_L} + r_1 e^{ikz_L}\right)\left(e^{ik(z_R - L} + r_2 e^{-ik(z_R - L)}\right)}{2ike^{-ikL}\left(1 - r_1 r_2 e^{2ikL}\right)}, \tag{11}$$

which together with Eq.(8) yields the momentum flowing within $\mathcal{V}$,

$$T_z^z = \frac{1}{\pi}\mathrm{Re}\int dE\, k\frac{1 + r_1 r_2 e^{2ikL}}{1 - r_1 r_2 e^{2ikL}} f(E), \tag{12}$$

which may be conveniently written as

$$T_z^z = \frac{\hbar^2}{\pi m}\mathrm{Re}\int dk\, k^2\frac{1 + r_1 r_2 e^{2ikL}}{1 - r_1 r_2 e^{2ikL}} f(E) \tag{13}$$

by using the relationship $E = \hbar^2 k^2/2m + V$ and changing integration variable. Notice that, as expected in an equilibrium situation, T_z^z is independent of z.

3. Three dimensional systems

The generalization of the results derived above to the three dimensional case is straightforward for systems which are translationally invariant along a symmetry plane, say xy. In that case, the parallel wave vector $\vec{Q} = (Q_x, Q_y)$ is a conserved quantity, and for each $\vec{Q}$ the problem is identical to the 1D case. Thus, we only have to sum Eq. (12) over the allowed wavevectors,

$$\mathcal{T}_z^z = \frac{\hbar^2}{4\pi^3 m}\mathrm{Re}\int d^2Q \int dk\, k^2\frac{1 + r_1 r_2 e^{2ikL}}{1 - r_1 r_2 e^{2ikL}} f(E) \tag{14}$$

where we introduced the number $\mathcal{A}d^2Q/(2\pi)^2$ of wavevectors within a region d^2Q of reciprocal space by applying Born-von Karman boundary conditions in a system with total area $\mathcal{A} \to \infty$, and we introduced the momentum flux *density* $\mathcal{T}_z^z = T_z^z/\mathcal{A}$. Notice that $-\mathcal{T}_z^z$ coincides with the zz component of the stress tensor as defined in elasticity theory.

We remark that the structure of Eq. (14) is essentially identical to Lifshitz's formula for the Casimir effect between two materials when written in terms of their optical reflection coefficients [12, 13]. The main differences are that the electromagnetic field has two independent transverse polarizations whose contributions would have to be summed over, and that the speed of light is a constant c, while the speed of electrons is proportional to the wavevector, i.e., the dispersion relation between electrons and photons are different, and consequently, there is an extra power of $\hbar$ in Eq. (14).

As r_1 and r_2 are independent of $\vec{Q}$ for scalar fields, the first integral in Eq. (14) may be performed immediately. At zero temperature we obtain

$$\mathcal{T}_z^z = \frac{1}{\pi^2}\mathrm{Re}\int dk\,\left(K_F - \frac{\hbar^2}{2m}k^2\right)k^2\frac{1+r_1r_2e^{2ikL}}{1-r_1r_2e^{2ikL}}, \tag{15}$$

where the integration region includes all states below the Fermi level, whose kinetic energy within $\mathcal{V}$ is K_F, and for which we took $f(E) = 2$, including the spin degeneracy.

4. Applications

4.1. One semiinfinite metal

Within the bulk of a semiinfinite metal the electrons are reflected by the surface potential barrier on one side, while there is no barrier on the other side. Thus, the pressure p with which the electrons push the surface of the metal may be obtained by setting $r_1 = 0$ in Eq. (15). The result is simply

$$p = \mathcal{T}_z^z = \frac{1}{\pi^2}\int_0^{k_F} dk\,\left(E_F - \frac{\hbar^2k^2}{2m}\right)k^2 = \frac{2}{5}nE_F, \tag{16}$$

where $\hbar k_F$ is the Fermi momentum, $E_F = K_F$ (within the metal) is the Fermi energy, and $n = k_F^3/3\pi^2$ is the electronic density. As could have been expected, this result coincides with the well known pressure of a degenerate fermion gas [17].

4.2. Two semiinfinite metals

We consider now two identical semiinfinite metals separated by vacuum. The force $F/\mathcal{A}$ per unit area between both metals may be obtained from the momentum flux (15) within the vacuum region, where the wavefunction of all the occupied states are evanescent, and it may be written as

$$\frac{F}{\mathcal{A}} = -2\mathrm{Im}\frac{\hbar^2}{2m\pi^2}\int_{\kappa_0}^{\kappa_F} d\kappa\,(\kappa_F^2 - \kappa^2)\kappa^2\frac{1}{\zeta - 1}, \tag{17}$$

where $\zeta^{-1} = r^2e^{-2\kappa L}$, and we wrote the wavenumber $k = i\kappa$ in terms of the decay constant κ. The integration limits in (17) are the decay constants for electrons at the bottom of the conduction band, $\kappa_0 = \sqrt{[}2m(W + E_F)/\hbar^2]$, and at the Fermi level $\kappa_F = \sqrt{(}2mW/\hbar^2)$, while $W = K_F$ (within vacuum) is the work function, and $r = r_1 = r_2$ is the complex reflection amplitude corresponding to evanescent

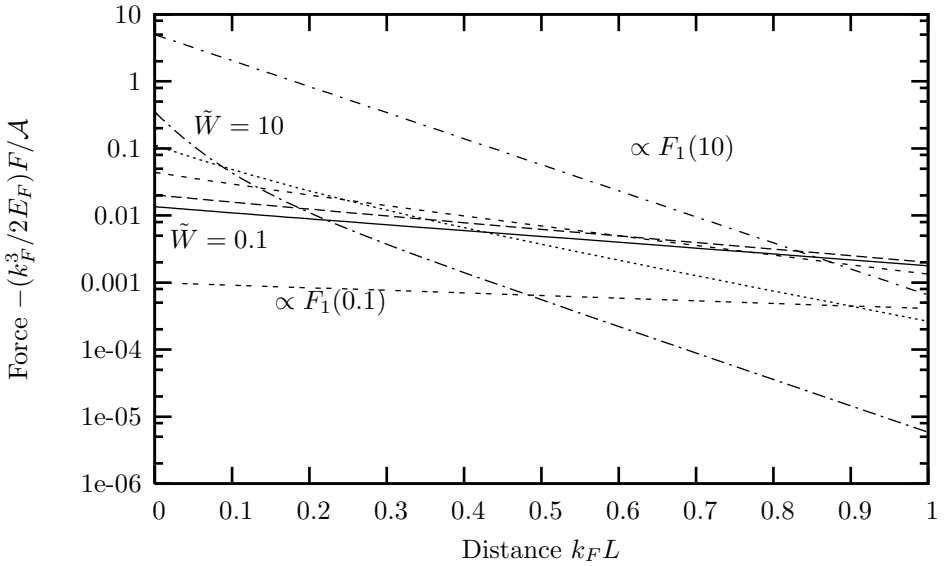

Figure 1. Force por unit area between two semiinfinite metals as function of their separation L for different values $0.1, 0.3, 1, 3, 10$ of the dimensionless work function $\tilde{W} = W/2E_F$. Also shown schematically is the contribution $e^{-2\kappa_F L} \propto F_1$ expected for one electron at the Fermi surface in the cases $\tilde{W} = 0.1, 10$.

wavefunctions that *propagate* (i.e., decay) through vacuum towards a surface and are reflected back. Assuming that the potential $V(z)$ is constant within the metals and within vacuum, and that it changes abruptly at the vacuum-metal interface by an amount $W+E_F$, the reflection amplitude may be calculated as $r = (i\kappa - k_M)/(i\kappa + k_M)$, where $k_M = \sqrt{[2m(W+E_F)/\hbar^2 - \kappa^2]}$ is the wavenumber within the metal of the state corresponding to κ.

In Fig. 1 we plot the force per unit area as a function of distance for different values of the workfunction W. The force is attractive, seems to decay exponentially for *large* separations and attains a finite value at zero separation. For large W the force is larger at small separation and smaller at large separations as the energy decays very fast towards that of two isolated semiinfinite metals. As could have been expected, the smaller the work function, the larger the spatial range of the force. We might expect the decay to be dominated by those electrons closest to the Fermi energy whose contribution becomes proportional to $e^{-2\kappa_F L}$. Fig. 1 includes two curves illustrating this behavior for the cases of large and small W. The actual decay of the force is slightly faster, more so for small W. This is due to the fact that not only the contribution of each electron decays with increasing distance, but also the number of electrons that contribute effectively to the force. Furthermore, the phase space available right at the Fermi energy is null, due to the prefactor $\kappa_F^2 - \kappa^2$ in Eq. (17), so the contributing electrons have a slightly larger decay constant (i.e., smaller range) than those at the Fermi level.

In Fig. 2 we show the force for several distances as a function of W. For finite separation distances the force is small when W is large, as the surfaces don't *feel* each other anymore, and it is also small for small workfunction, as the electrons tunnel too easily between the two metals, not *caring* about the separation. Thus, the magnitude

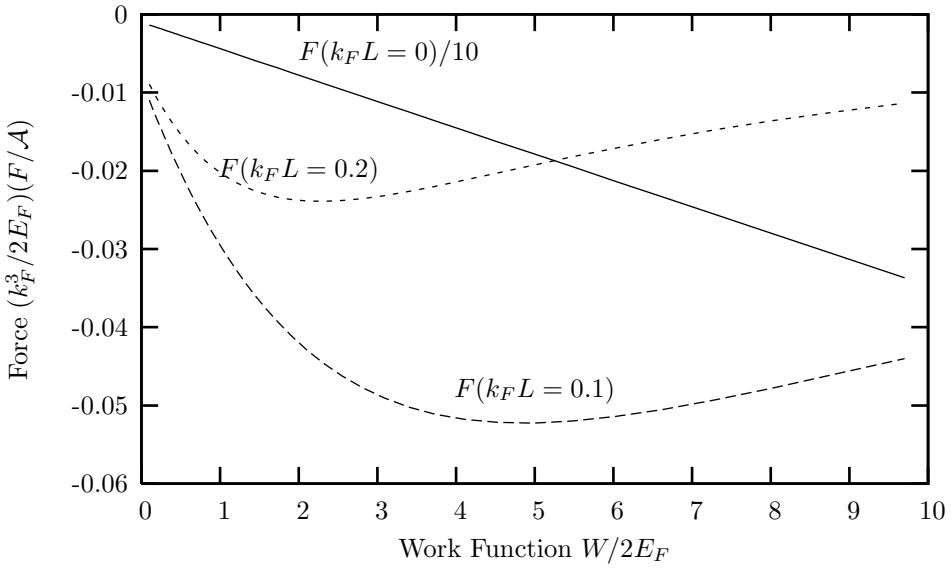

Figure 2. Force between two metals as a function of the work function for several values of the separation $\tilde{L} = 0, 0.1, 0.2$ in units of k_F^{-1}.

of the force is largest at some intermediate value of W which increases as L decreases. At contact, $L = 0$, there is no such extreme anymore and we obtain a linear behavior,

$$\frac{F(0)}{\mathcal{A}} = -\frac{q_F^3}{\pi^2}\left(\frac{E_F}{5} + \frac{W}{3}\right), \tag{18}$$

as can be shown by integrating Eq. (17) analytically. $F(0)$ is the force that would be required in order to break an infinite metal into two semiinfinite ones. Eq. (18) actually overestimates the ultimate breaking strength of real materials by several orders of magnitude as our model fails to account for dislocations whose motion within the metal would relax the stress, and for the growth of fractures which are actually responsible for the failure of real metals. Real metals break gradually, not simultaneously over the whole separation surface. Nevertheless, integrating Eq. (17) over L we have obtained an analytical estimate of the surface energy of metals in terms only of their Fermi energy and their work function. This turns out to be surprisingly accurate [18] given our simplifying assumptions, namely, our use of an independent free particle model, neglecting the crystalline structure, the electronic charge, and many body corrections, as well as our use of a square potential barrier at the surface.

5. Thin films

Eq. (17) may be employed to calculate the force between more complicated systems simply by introducing the appropriate value of the reflection amplitude. For example, in Fig. 3 we display the force between two free standing very thin metallic films as a function of distance for a fixed Fermi energy, or more properly, a fixed electrochemical potential. Notice that for very thin films the force is identically zero, as there are no states at all below the Fermi energy and therefore there are no available electrons to tunnel between the films. For wider films the force is finite at small separations but

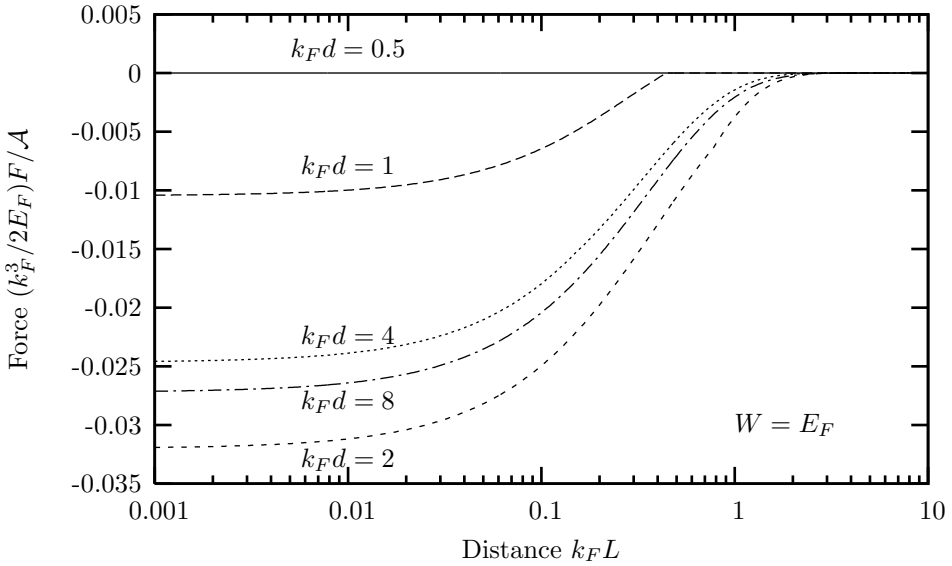

Figure 3. Force between two films of widths $\tilde{d} = 0.5, 1, 2, 4, 8$ (in units of k_F^{-1}) as a function of the distance L between them. We took $W = E_F$.

becomes zero after a finite separation. As the width is further increased, the force approaches that corresponding to semiinfinite metals, although not monotonously; it actually oscillates between larger and smaller values. This behavior may be understood by considering the finite size effect on the levels of the individual films, and the interaction of levels within both films, yielding alternating bonding and antibonding states which may be occupied only when they lie below the Fermi level.

6. Conclusions

By calculating the mechanical properties carried by the electronic wavefunctions, we have shown that the interchange of electrons between conductors produces a force that may be calculated in terms of the electronic reflection amplitudes using formulae that are very closely related to Lifshitz formula for the usual Casimir force. We illustrated our formalism by calculating the electronic pressure within a conductor and the force between semiinfinite conductors and between thin films at very small distances, of the order of the Fermi wavelength. These distances are extremely small, beyond the expected limit of validity of the usual Casimir effect. Thus, we expect our results to be important to study the forces that act, for example, between the tip and the substrate of a scanning tunneling microscope [19]. We discussed how our results may be employed to calculate the surface energy of conductors without having to substract total energies. Other applications which are currently under study include the calculation of the force between impurities embedded within three and one-dimensional conductors. Although our current calculations were performed for free, independent electron conductors, we believe that our scattering approach might be generalized to more realistic systems of interacting electrons.

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Bibliography

[1] Lamoreaux S K 1997 *Phys. Rev. Lett.* **78** 5; Lamoreaux S K and Buttler W T 2005 *Phys. Rev.* E **71** 036109
[2] Mohideen U and Roy A 1998 *Phys. Rev. Lett.* **81**, 4549; Harris B W, Chen F and Mohideen U 2000 *Phys. Rev.* A **62** 052109; Chen F, Klimchitskaya G L, Mohideen U and Mostepanenko V M 2004 *Phys. Rev.* A **69** 022117; Chen F, Mohideen U, Klimchitskaya G L and Mostepanenko V M 2005 *Phys. Rev.* A **72** 020101
[3] Chan H B, Aksyuk V A, Kliman R N, Bishop D J and Capasso F 2001 *Science* **291** 1942
[4] Decca RS, Lopez D, Fischbach E and Krause D E 2003 *Phys. Rev. Lett.* **91** 050402; Decca R S, Lopez D, Fischbach E, Klimchitskaya G L, Krause D E and Mostepanenko V M 2005, *Ann. of Phys.* **318** 37
[5] Bressi G, Carugno G, Onofrio R and Ruoso G 2002 *Phys. Rev. Lett.* **88** 041804
[6] Casimir H B G 1948 *Proc. Kon. Ned. Akad. Wet.* **51** 793
[7] Iannuzzi D, Lisanti M and Capasso F 2004 *Proc. Natl. Acad. Sci.* **101** 4019
[8] Munday J N, Iannuzzi D, Barash Y and Capasso F 2005 *Phys. Rev.* A **71** 042102; Torres-Guzmán J C and Mochán W L (submitted to J. Phys. A)
[9] Serry F M, Walliser D, and Maclay G J 1998 *J. Appl. Phys.* **84** 2501
[10] Esquivel-Sirvent R, Villarreal C and Cocoletzi G H 2001 *Phys. Rev.* A **64** 052108; Villarreal C, Esquivel-Sirvent R and Cocoletzi G H 2002 *Int. J. of Mod. Phys.* A *17* 798; Esquivel-Sirvent R, Villarreal C, Mochán W L and Cocoletzi GH 2002 *Phys. Stat. Sol.* (b) **230** 409
[11] Krause D E and Fischbach E 2002 *Phys. Rev. Lett.* **89** 190406; Decca R S, Fischbach E, Klimchitskaya GL, Krause D E, Lopez D and Mostepanenko V M 2003 *Phys. Rev.* D **68** 11603
[12] Jaekel M T and Reynaud S 1991 *J. Phys.* **1** 1395; Genet C, Lambrecht A and Reynaud S 2003 *Phys. Rev.* A **67** 043811
[13] Mochán W L, Villarreal C and Esquivel-Sirvent R, 2002 *Rev. Mex. Fis.* **48** 339; Esquivel-Sirvent R, Villarreal C and Mochán W L 2003 *Phys. Rev.* A **68** 052103; Esquivel-Sirvent R, Villarreal C and Mochán W L 2005 *Phys. Rev.* A **71**, 029904; Mochán W L, Contreras-Reyes A M, Esquivel-Sirvent R and Villarreal C 2005 *Statistical Physics and Beyond: 2nd Mexican Meeting on Mathematical and Experimental Physics* ed F J Uribe *et al.* (AIP Conference Proceedings) (Melville: American Institute of Physics) p 66
[14] Lifshitz E M 1956 *Sov. Phys. JETP* **2** 73; Barash Y and Ginzburg VL 1975 *Sov. Phys.-Usp.* **18** 305
[15] Goldstein H 1950 *Classical Mechanics*, (Reading: Addison-Wesley Publishing Co.)
[16] Bogoliubov N N and Shirkov D V 1979 *Introduction to the Theory of Quantized Fields* (New York: John Wiley and Sons)
[17] Pathria R K 1972 *Statistical Mechanics* (Oxford: Pergamonn Press)
[18] Procopio LM, Villarreal C and Mochán WL, unpublished
[19] Iannuzzi D, personal communication; Mohideen U, personal communication